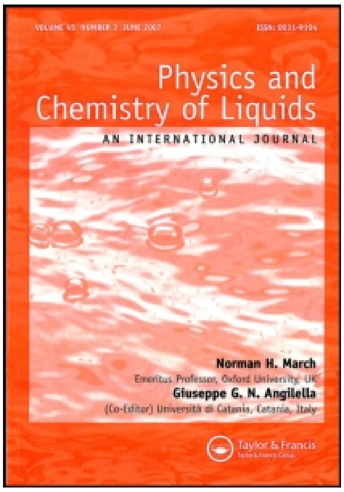

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The sound velocities in dense fluids from distribution functions

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The sound velocities in dense fluids from distribution functions

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The sound velocities and adiabatic compressibilities in dense fluids have been evaluated using three known analytical expressions for radial distribution functions (RDFs). Using such approach not only tests the power of distribution functions theory in predicting the sound velocities and adiabatic compressibilities, but also specifies better expressions in determining these properties. To calculate these quantities, the variation of RDF with density and temperature is required. Therefore, we should have analytical expressions which explicitly present RDF as a function of temperature, density and interparticle distance. It is shown that if an expression is used which properly presents RDFs as a function of interparticle distance, density and temperature, it is possible to calculate sound velocities and adiabatic compressibilities from distribution function theory.

Keywords: radial distribution function; sound velocities; adiabatic compressibilities; statistical mechanics

1. Introduction

The radial distribution function (RDF) acts as a bridge for relating macroscopic thermodynamic properties to interparticle interactions of substances. The RDF is a key quantity in statistical mechanics because it characterises how the particles correlates in a substance decay with increasing separation [1].

Among the quantities being of high importance are the sound velocities [2], which have been extensively tabled for different substances and mixtures [3–10]. The sound velocities in fluids are related to different thermodynamic properties such as molecular weight [11], molecular radius [12], surface tension [13], structure and dynamics of interface [14], boiling and critical points, molecular refraction, Souders viscosity constant, van der Waals, b, molecular magnetic rotation [15], pseudo-Gruneisen parameters [16] and intermolecular free length [17].

Analytical expressions for RDFs have most often been used for the evaluation of pressure and internal energy [18–21]. In previous cases as a substitute method, RDFs could have directly been obtained as a function of distance using molecular dynamics (MD) or integral equations. Recently, these expressions have been used for the evaluation of $P-V-T$ differential properties, such as internal pressure, thermal pressure and isothermal compressibility [22].

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In this work, sound velocities and adiabatic compressibilities are evaluated using three known analytical expressions for RDFs [18–20]. For the evaluation of sound velocities and adiabatic compressibilities, differentials like $(\partial g(r,\rho,T)/\partial\rho)_{r,T}$ and $(\partial g(r,\rho,T)/\partial T)_{r,\rho}$ are required where $g(r,\rho,T)$, r, ρ and T are RDF, interparticle distance, density and temperature, respectively. This problem shows our requirement for analytical expressions which explicitly presents RDFs as a function of r, ρ and T.

Until now, this approach (using distribution functions theory) has not been utilised to estimate the values of sound velocities and adiabatic compressibilities.

Using such approach not only tests the power of distribution functions theory in predicting the sound velocities and adiabatic compressibilities, but also specifies better equations in determining these properties.

The results are compared with experimental data for argon [23] and an accurate analytic equation of state for the LJ fluid [24].

2. Theory

2.1. *Statistical mechanical equations for sound velocity and adiabatic compressibility*

It can be illustrated that the velocity of sound (c) propagated through a fluid is [25]

$$c^2 = \frac{1}{m}\left(\frac{\partial P}{\partial \rho}\right)_S, \tag{1}$$

where c, S and m are velocity of sound, entropy and mass of one atom, respectively.

For Fluids, the expression $(\partial P/\partial\rho)_S$ for the sound velocity is often written as

$$c = \left(\frac{1}{m\kappa_S\rho}\right)^{1/2}, \tag{2}$$

where κ_S is adiabatic compressibility.

Since

$$\kappa_S = \frac{1}{\rho}\left(\frac{\partial \rho}{\partial P}\right)_S, \tag{3}$$

we have

$$\kappa_S^{-1} = \kappa_T^{-1} + \frac{T}{\rho}\frac{(\partial P/\partial T)_V^2}{C_V}, \tag{4}$$

where κ_T and C_V are isothermal compressibility and heat capacity at constant volume, respectively.

The temperature dependence of the internal energy (E) is given by the heat capacity at constant volume (C_V) at a given temperature, formally defined by

$$C_V = \left(\frac{\partial E}{\partial T}\right)_V, \tag{5}$$

where $V = 1/\rho$ is molar volume.

Consider a system of N particles. Since

$$E = E^{\mathrm{ig}} + 2\pi N\rho \int_0^\infty u(r)g(r,\rho,T)r^2 \mathrm{d}r, \tag{6}$$

where E^{ig} and $u(r)$ are internal energy for ideal gas and interparticle pair potential, respectively, we have

$$C_V = \frac{3}{2}Nk + 2\pi N\rho \int_0^\infty u(r)\left(\frac{\partial g(r,\rho,T)}{\partial T}\right)_{r,T} r^2 \mathrm{d}r. \tag{7}$$

Isothermal compressibility is defined as

$$\kappa_T = \frac{1}{\rho}\left(\frac{\partial \rho}{\partial P}\right)_T, \tag{8}$$

since

$$P = \rho kT - \frac{2\pi}{3}\rho^2 \int_0^\infty \frac{\mathrm{d}u(r)}{\mathrm{d}r} g(r,\rho,T)r^3 \mathrm{d}r, \tag{9}$$

where k is the Boltzmann's constant, we have

$$\kappa_T^{-1} = \rho kT - \frac{2\pi}{3}\rho^2 \int_0^\infty \frac{\mathrm{d}u(r)}{\mathrm{d}r}\left\{2g(r,\rho,T) - \rho\left(\frac{\partial g(r,\rho,T)}{\partial \rho}\right)_{r,T}\right\} r^3 \mathrm{d}r, \tag{10}$$

and

$$\left(\frac{\partial P}{\partial T}\right)_V = \rho k - \frac{2\pi}{3}\rho^2 \int_0^\infty \frac{\mathrm{d}u(r)}{\mathrm{d}r}\left(\frac{\partial g(r,\rho,T)}{\partial T}\right)_{r,\rho} r^3 \mathrm{d}r. \tag{11}$$

2.2. *The known expressions for RDF of a LJ fluid*

2.2.1. *Goldman expression*

An expression for the RDF of an LJ fluid was introduced by Goldman [18] in 1979. The expression is

$$g(r^*) = g_a(r^*) + g_b(r^*) + g_c(r^*), \tag{12}$$

where

$$g_a(r^*) = 0 \quad r^* \le B_1, \tag{13}$$

$$g_a(r^*) = \frac{B_2}{r^* - B_1}\exp(-[B_3\{\ln(r^* - B_1) + B_4\}^2]) \quad r^* > B_1, \tag{14}$$

$$g_b(r^*) = c\exp\left(-\frac{u(r^*)}{kT}\right) \quad r^* \le B_9, \tag{15}$$

$$g_b(r^*) = \exp\left(-\frac{[r^* - B_5]^2}{B_6}\right) \quad B_9 \le r^* \le B_5, \tag{16}$$

$$g_b(r^*) = 1 \quad r^* > B_5, \tag{17}$$

$$g_c(r^*) = 0 \quad r^* \le B_5 - 0.25B_7, \tag{18}$$

$$g_c(r^*) = \exp(-B_8 r^*) \sin\left[\frac{2\pi(r^* - B_5 + 0.25B_7)}{B_7}\right] \quad r^* > B_5 - 0.25B_7, \tag{19}$$

where $r^* = r/\sigma$, $T^* = kT/\varepsilon$ and $\rho^* = \rho\sigma^3$ are reduced interparticle distance, reduced temperature and reduced density, respectively. $k, \sigma, \varepsilon, r, T$ and ρ are the Boltzmann constant, length parameter of a potential function, energy parameter of a potential function, interparticle distance, absolute temperature and density, respectively. B_1–B_9 and C are adjustable parameters being functions of temperature and density [18]. These parameters have been presented as polynomials in ρ^* and T^*, using 108 constants. This expression is valid within $0.5 \le T^* \le 5.1$ and $0.35 \le \rho^* \le 1.1$.

2.2.2. *Matteoli and Mansoori expression*

Matteoli and Mansoori [19] have derived an expression for RDF of a LJ fluid as the followings:

$$g(y) = 1 + y^{-m}[g(d) - 1 - \lambda] + \left[\frac{(y - 1 + \lambda)}{y}\right]\{\exp[-\alpha(y-1)]\cos[\beta(y-1)]\}$$
$$m \ge 1, \quad y \ge 1, \tag{20}$$

$$g(y) = g(d)\exp[-\theta(y-1)^2], \quad y < 1 \tag{21}$$

where $y = r/h\sigma$ is dimensionless interparticle distance and h, m, λ, α and β are adjustable parameters being functions of temperature and density. These parameters have been expanded in terms of ρ^* and T^*, using 21 constants. This expression is valid within $0.6 \le T^* \le 3.7$ and $0.35 \le \rho^* \le 0.9$. In this article, this expression is referred as MM expression.

2.2.3. *Morsali* et al. *expression*

Morsali *et al.* [20] derived the following expression for RDF of a LJ fluid:

$$g(r^*) = 1 + (r^*)^{-2}\exp[-(ar^* + b)]\sin[(cr^* + d)]$$
$$+ (r^*)^{-2}\exp[-(gr^* + h)]\cos[(kr^* + l)] r^* > 1, \tag{22}$$

$$g(r^*) = s\exp[-(mr^* + n)^4], \tag{23}$$

where a, b, c, d, g, h, k, l, s, m and n are adjustable parameters being functions of temperature and density. These parameters have been expanded in terms of ρ^* and T^*, using 65 constants. This expression is valid within $0.5 \leq T^* \leq 5.1$ and $0.35 \leq \rho^* \leq 1.1$. This expression is referred hereafter as MGMA expression.

3. Results and discussion

The values of c, κ_S, κ_T and C_V should be expressed in their reduced form in order to calculate them as functions of reduced density, ρ^* and reduced temperature, T^*:

$$c^* = c\left(\frac{m}{\varepsilon}\right)^{1/2}, \quad \kappa_S^* = \frac{\kappa_S \varepsilon}{\sigma^3}, \quad \kappa_T^* = \frac{\kappa_T \varepsilon}{\sigma^3}, \quad C_V^* = \frac{C_V}{Nk}, \tag{24}$$

The reduced form for $u(r), P, E, C_V, (\partial P/\partial T)_\rho, \kappa_T, \kappa_S$ and c are

$$u(r^*) = 4[(r^*)^{-12} - (r^*)^{-6}], \tag{25}$$

$$P^* = \rho^* T^* - 16\pi(\rho^*)^2 \int_0^\infty g(r^*) \times [(r^*)^{-4} - 2(r^*)^{-10}]\mathrm{d}r^*, \tag{26}$$

$$E^* = \frac{3}{2}T^* + 8\pi\rho^* \int_0^\infty [(r^*)^{-10} - (r^*)^{-4}]g(r^*, \rho^*, T^*)\mathrm{d}r^*, \tag{27}$$

$$C_V^* = \frac{3}{2} + 8\pi\rho^* \int_0^\infty [(r^*)^{-10} - (r^*)^{-4}]\frac{\partial g(r^*, \rho^*, T^*)}{\partial T^*}\mathrm{d}r^*, \tag{28}$$

$$\left(\frac{\partial P^*}{\partial T^*}\right)_{\rho^*} = \rho^* - 16\pi(\rho^*)^2 \int_0^\infty [(r^*)^{-4} - (r^*)^{-10}]\left(\frac{\partial g(r^*, \rho^*, T^*)}{\partial T^*}\right)_{r^*, \rho^*} \mathrm{d}r^*, \tag{29}$$

$$\begin{aligned}(\kappa_T^*)^{-1} = T^*\rho^* - 16\pi(\rho^*)^2 \int_0^\infty [(r^*)^{-4} - (r^*)^{-10}] \\ \times \left\{2g(r^*, \rho^*, T^*) + \rho^*\left(\frac{\partial g(r^*, \rho^*, T^*)}{\partial \rho^*}\right)_{r^*, T^*}\right\}\mathrm{d}r^*,\end{aligned} \tag{30}$$

$$\left(\kappa_S^*\right)^{-1} = \left(\kappa_T^*\right)^{-1} + \frac{T^*}{\rho^*}\frac{(\partial P^*/\partial T^*)^2_{\rho^*}}{C_V^*}, \tag{31}$$

$$c^* = \left(\frac{1}{\kappa_S^* \rho^*}\right)^{1/2}. \tag{32}$$

Using Equations (24)–(32) and Goldman, MM and MGMA expressions, theoretical values of κ_S^* and c^* are obtained. These quantities are compared with Kolafa and Nezbeda equation of state (KN EOS) [24] and experimental data (Exp.) [23]. Experimental data (Argon) has been converted to reduced format using $\sigma = 3.405$ Å and $\varepsilon/k = 119.8$ K.

The equations related to KN EOS are as follows:

$$\frac{P^*}{\rho^* T^*} = z_{HS} + \rho(1 - 2\gamma\rho^{*2})\exp(-\gamma\rho^{*2})\Delta B_{2,hBH} + \sum_{ij} jC_{ij}(T^*)^{i/2-1}(\rho^*)^j, \quad (33)$$

$$E^* = \frac{3(z_{HS} - 1)}{d_{hBH}}\frac{\partial d_{hBH}}{\partial(1/T^*)} + \rho\exp(-\gamma\rho^{*2})\frac{\partial \Delta B_{2,hBH}}{\partial(1/T^*)} - \sum_{ij}(i/2-1)C_{ij}(T^*)^{i/2}(\rho^*)^j, \quad (34)$$

where z_{HS} is

$$z_{HS} = \frac{P^*_{HS}}{\rho^* T^*} = \frac{1 + \eta + \eta^2 - \eta^3(2/3)(1+\eta)}{(1-\eta)^3}, \quad (35)$$

with $\eta = \pi(\rho^*)^3 d^3_{hBH}/6$. Functions d_{hBD} and $\Delta B_{2,hDB}$ are approximated by the following equation with coefficients given in [14]:

$$f(T^*) = \sum_i C_i T^{*\,i/2} + C_{\ln}\ln(T^*); \quad f(T^*) = (d_{hBH}, \Delta B_{2,hBH}), \quad (36)$$

d_{hBD} and $\Delta B_{2,hDB}$ derivatives over $1/T$ are

$$\frac{\partial f(T^*)}{\partial(1/T^*)} = -T^*\left(\sum_i \frac{i}{2} C_i T^{*\,i/2} + C_{\ln}\right). \quad (37)$$

The reduced sound velocities and adiabatic compressibilities have been calculated using three expressions for RDFs of a LJ fluid at reduced temperature, $T^* = 1.002, 1.502, 1.669, 2.087, 2.504, 2.922, 3.339, 3.756, 4.174, 4.674, 5.008$ and reduced densities, $0.357 \le \rho^* \le 1.1$ (177 points altogether) and compared with those of EOS and experimental data. Although range of validity of Goldman equation $0.5 \le T^* \le 5.1$ and $0.35 \le \rho^* \le 1.1$ has been reported, care should be taken when it is applied at high temperatures and low densities [22]. Also, due to range of validity of MM expression, $T^* = 3.756$–5.008 has been omitted (113 points altogether).

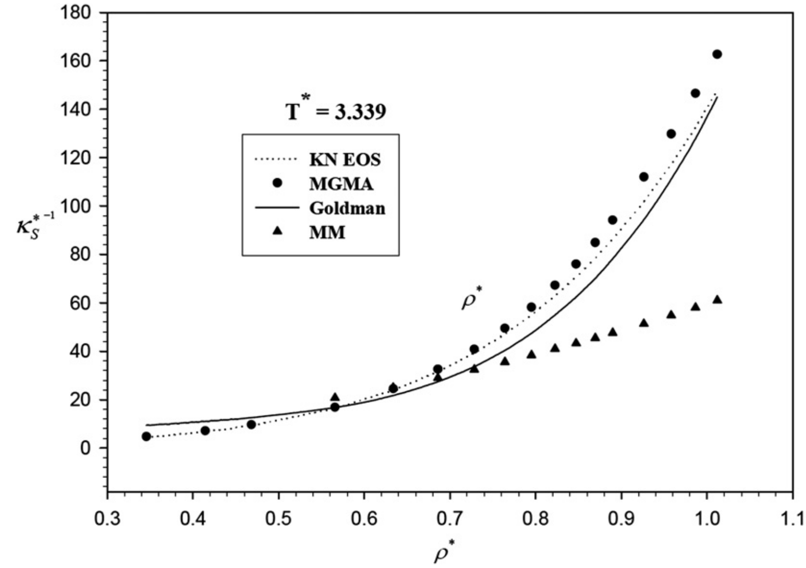
Therefore, initially the sound velocities and adiabatic compressibilities are evaluated at reduced temperatures of 1.002–3.339 (113 points altogether). Figure 1 demonstrates $(\kappa^*_S)^{-1}$ *versus* ρ^* at $T^* = 2.087, 3.339$. In this figure, theoretical values obtained from Goldman, MM and MGMA expressions have been compared with those of KN EOS. Table 1 shows the numerical values of $(\kappa^*_S)^{-1}$ at reduced temperatures $T^* = 1.502, 1.669$ and different densities.

If KN EOS is taken as the criteria for comparison, the values of average absolute deviations (AAD)

$$\left(\text{AAD} = \frac{1}{n}\sum_{i=1}^{n} 100 \times \frac{\left|\left(\kappa^*_{S,i}\right)^{-1}_{\text{KN EOS}} - \left(\kappa^*_{S,i}\right)^{-1}_{\text{theory}}\right|}{\left(\kappa^*_{S,i}\right)^{-1}_{\text{KN EOS}}}\right),$$

related to $(\kappa^*_S)^{-1}$ in connection with Goldman, MM and MGMA expressions at range of applied temperatures and densities are 8.40, 40.13 and 5.07, respectively.

Figure 2 demonstrates c^* *versus* ρ^* at $T^* = 2.087, 3.339$. In this figure, theoretical values obtained from Goldman, MM and MGMA expressions have been compared with



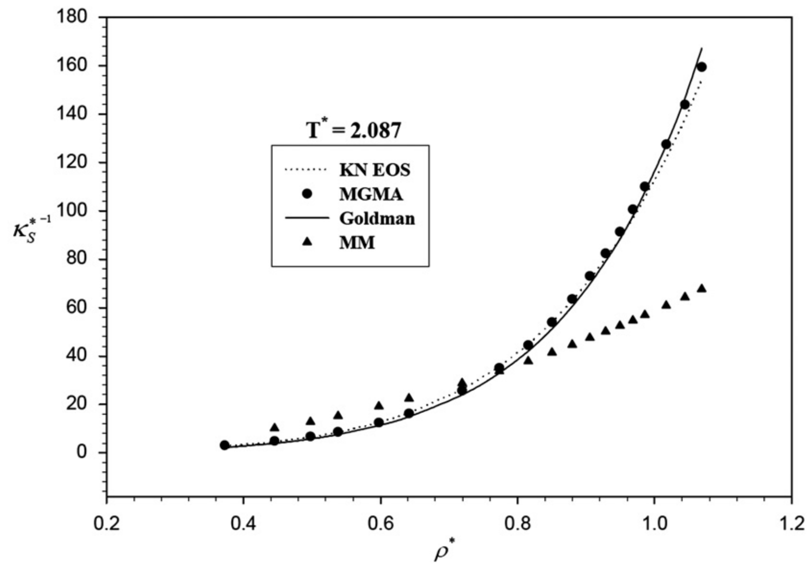


Figure 1. $(\kappa_S^*)^{-1}$ *vs.* ρ^* at $T^* = 2.087,\ 3.339$. Theoretical values obtained from Goldman (—), MM (▲) and MGMA (●) expressions have been compared with those of KN EOS (•••).

those of KN EOS and experimental data (Exp.). Table 1 shows the numerical values of c^* at reduced temperatures $T^* = 1.502,\ 1.669$ and different densities.

If KN EOS (Exp.) is taken as the criteria for comparison, the AAD values related to c^*

$$\left(\mathrm{AAD} = \frac{1}{n}\sum_{i=1}^{n} 100 \times \frac{\left|c^*_{i,\mathrm{KN\,EOS(Exp.)}} - c^*_{i,\ \mathrm{theory}}\right|}{c^*_{i,\ \mathrm{KN\,EOS(Exp.)}}}\right),$$

Table 1. Comparison of numerical values of $(\kappa_S^*)^{-1}$ and c^* at $T^* = 1.502,\ 1.669$.

T^*	ρ^*	$(\kappa_S^*)^{-1}_{\text{KN EOS}}$	$(\kappa_S^*)^{-1}_{\text{MGMA}}$	$(\kappa_S^*)^{-1}_{\text{Goldman}}$	$(\kappa_S^*)^{-1}_{\text{MM}}$	$c^*_{\text{Exp.}}$	$c^*_{\text{KN EOS}}$	c^*_{MGMA}	c^*_{Goldamn}	c^*_{MM}
1.502	0.684	15.690	15.070	15.601	22.816	4.657	4.789	4.694	4.776	5.775
1.502	0.725	20.701	19.520	20.036	26.372	5.195	5.344	5.189	5.257	6.031
1.502	0.757	25.444	23.783	24.291	29.335	5.632	5.798	5.605	5.665	6.225
1.502	0.816	36.419	33.906	34.463	35.220	6.481	6.681	6.446	6.499	6.570
1.502	0.860	46.805	43.840	44.564	39.959	7.216	7.377	7.140	7.199	6.816
1.502	0.895	56.641	53.543	54.571	43.939	7.818	7.955	7.735	7.809	7.007
1.502	0.924	65.997	62.999	64.475	47.375	8.338	8.451	8.257	8.353	7.160
1.502	0.949	75.049	72.310	74.396	50.438	8.813	8.893	8.729	8.854	7.290
1.502	0.972	84.276	81.916	84.827	53.339	9.244	9.311	9.180	9.342	7.408
1.502	0.992	93.079	91.132	95.051	55.924	9.637	9.687	9.585	9.789	7.508
1.502	1.010	101.688	100.142	105.279	58.302	10.010	10.034	9.957	10.210	7.598
1.669	0.461	3.478	3.958	3.918	9.130	2.401	2.747	2.930	2.915	4.450
1.669	0.473	3.807	4.270	4.267	9.722	2.775	2.837	3.004	3.003	4.534
1.669	0.513	5.147	5.525	5.632	11.860	3.098	3.168	3.282	3.313	4.808
1.669	0.569	7.798	7.972	8.186	15.281	3.611	3.702	3.743	3.793	5.182
1.669	0.608	10.326	10.277	10.531	17.958	4.023	4.121	4.111	4.162	5.435
1.669	0.608	10.326	10.277	10.531	17.958	4.023	4.121	4.111	4.162	5.435
1.669	0.639	12.825	12.544	12.811	20.257	4.365	4.480	4.431	4.477	5.630
1.669	0.686	17.598	16.871	17.132	24.030	4.929	5.065	4.959	4.997	5.919
1.669	0.745	25.611	24.218	24.445	29.246	5.392	5.863	5.701	5.728	6.266
1.669	0.787	32.967	31.107	31.312	33.279	6.304	6.472	6.287	6.308	6.503
1.669	0.834	43.137	40.898	41.122	38.100	7.020	7.192	7.003	7.022	6.759
1.669	0.871	52.811	50.488	50.819	42.121	7.628	7.787	7.614	7.638	6.954
1.669	0.902	62.208	60.034	60.585	45.641	8.160	8.305	8.158	8.196	7.113
1.669	0.928	71.108	69.246	70.143	48.700	8.636	8.754	8.638	8.694	7.244
1.669	0.952	80.239	78.821	80.245	51.608	9.066	9.181	9.099	9.181	7.363
1.669	0.973	89.024	88.104	90.231	54.221	9.465	9.565	9.516	9.630	7.465
1.669	0.991	97.203	96.761	99.745	56.511	9.839	9.904	9.881	10.032	7.551
1.669	1.009	106.037	106.074	110.237	58.846	10.188	10.251	10.253	10.452	7.637
1.669	1.025	114.492	114.894	120.466	60.962	10.511	10.569	10.587	10.841	7.712

in connection with Goldman, MM and MGMA expressions at the range of applied temperatures and densities are 4.08(3.64), 20.49(20.68) and 2.50(4.41), respectively.

As it is seen from Figures 1 and 2 and Table 1, Goldman and MGMA expression well predict the values of $(\kappa_S^*)^{-1}$ and c^*, both quantitatively and qualitatively, but MM expression is accompanied with many errors, both quantitatively and qualitatively.

The above mentioned description was related to temperatures $1.002 \le T^* \le 3.339$. Goldman's expression is not able to reproduce RDFs well at high temperatures and low densities. The MM expression does not apply at temperatures $3.756 \le T^* \le 5.008$ and the Goldman's expression should be used with caution [22]. Therefore, for temperatures within the range of $3.756 \le T^* \le 5.008$, only the errors related to MGMA expression are reported.

Figure 3 demonstrates $(\kappa_S^*)^{-1}$ *versus* ρ^* and c^* *versus* ρ^* at $T^* = 4.174$. In this figure, theoretical values obtained from Goldman and MGMA expressions have been compared with those of KN EOS and experimental data (for c^*).

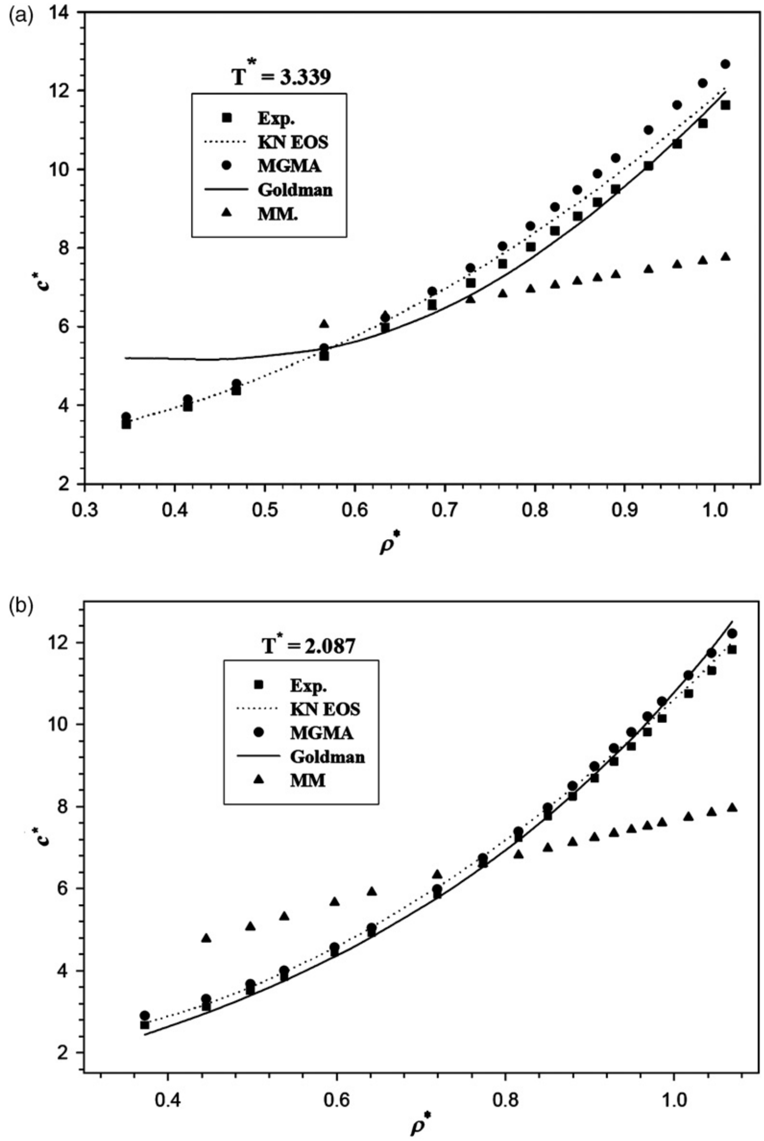


Figure 2. c^* *vs.* ρ^* at $T^* = 2.087,\ 3.339$. Theoretical values obtained from Goldman (—), MM (▲) and MGMA (●) expressions have been compared with those of KN EOS (•••) and Exp. (■).

For temperatures within the range of $3.756 \leq T^* \leq 5.008$, if KN EOS is taken as the criteria for comparison, the AAD value related to $(\kappa_{S,i}{}^*)^{-1}$

$$\left(\mathrm{AAD} = \frac{1}{n}\sum_{i=1}^{n} 100 \times \frac{\left|\left(\kappa^*_{S,i}\right)^{-1}_{\mathrm{KN\,EOS}} - \left(\kappa^*_{S,i}\right)^{-1}_{\mathrm{MGMA}}\right|}{\left(\kappa^*_{S,i}\right)^{-1}_{\mathrm{KN\,EOS}}}\right),$$

in connection with MGMA expressions is 4.31.

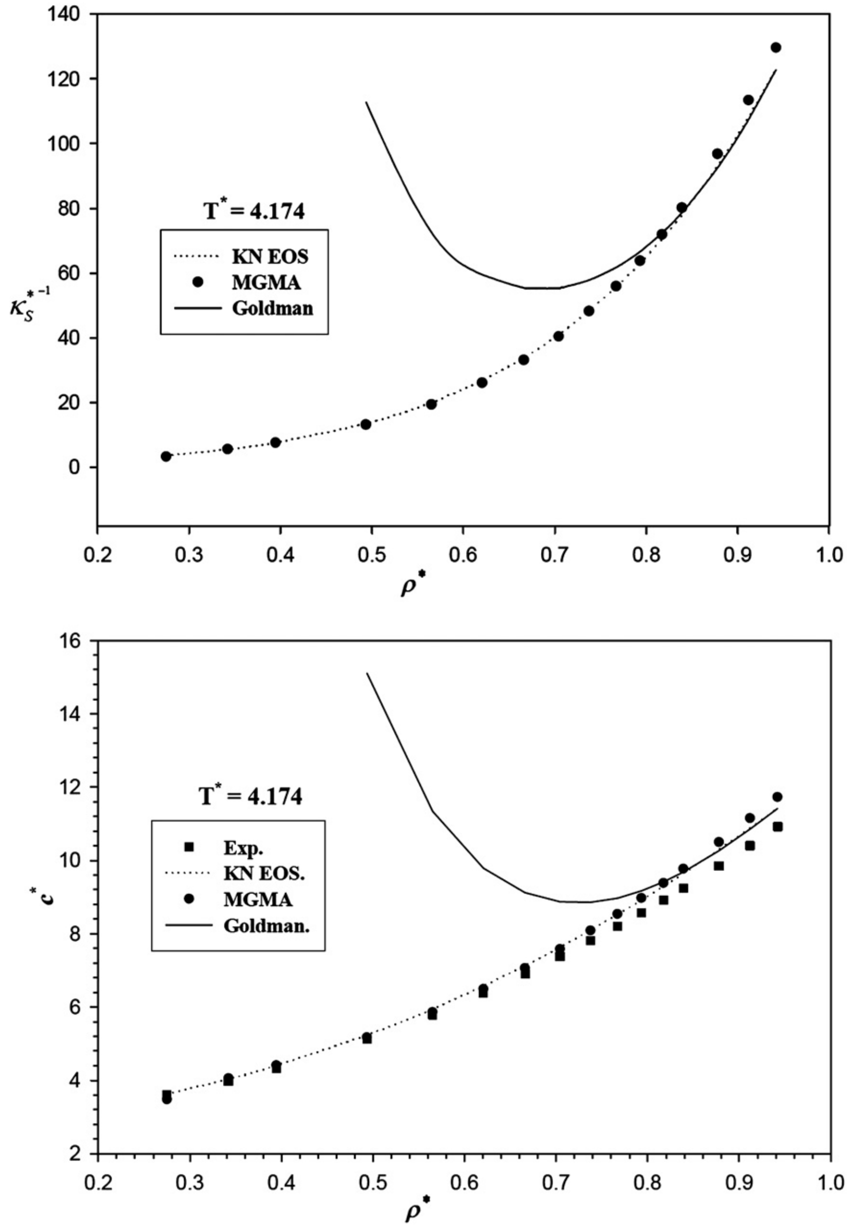


Figure 3. $(\kappa_S^*)^{-1}$ *vs.* ρ^* and c^* *vs.* ρ^* at $T^* = 4.174$. Theoretical values obtained from Goldman (—), MM (▲) and MGMA (●) expressions have been compared with those of Exp. (■) (for c^*) and KN EOS (•••).

If KN EOS (Exp.) is taken as the criteria for comparison, the AAD value related to c^*

$$\left(\mathrm{AAD} = \frac{1}{n}\sum_{i=1}^{n} 100 \times \frac{\left|c^*_{i,\mathrm{KN\,EOS(Exp.)}} - c^*_{i,\,\mathrm{theory}}\right|}{c^*_{i,\mathrm{KN\,EOS(Exp.)}}}\right),$$

in connection MGMA expressions at the range of applied temperatures ($3.756 \leq T^* \leq 5.008$) and densities is 2.51(3.43).

In general, the MGMA expression well predicts the quantities of $(\kappa_S^*)^{-1}$ and c^* within all ranges of temperatures and densities.

4. Conclusion

By using RDF theory, the sound velocities and adiabatic compressibilities were calculated. Three analytical expressions were used for this purpose which presents RDFs as a function of r, ρ and T. Within the range of lower temperatures, the Goldman and MGMA expressions both predict the values of $(\kappa_S^*)^{-1}$ and c^* with acceptable errors, but MM expression is not suitable for this purpose.

The MM expression does not apply at temperatures $3.756 \leq T^* \leq 5.008$ and the Goldman's expression should be used with caution. Within this range, the MGMA expression still well predicts the values of $(\kappa_S^*)^{-1}$ and c^*. The reason for this, besides more accuracy of MGMA expression in the reproducing of RDFs (rmsd: 0.025 *versus*. 0.034), is attributable to the number of parameters in these two expressions (65 *versuss*. 108). Because of the high number of parameters in Goldman expression, differentiation of this expression causes more errors.

Therefore, if an expression that presents $g(r)$ as a function of r, ρ and T is used, it is possible to calculate the sound velocities and adiabatic compressibilities from RDFs.

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References

[1] D.A. McQaarrie, *Statistical Mechanics* (Harper & Row, New York, 1975).
[2] H.N.V. Temperley, J.S. Rowlinson, and G.S. Ruhbrooke, *Physics of Simple Liquids* (North Holland Publishing Company, Amsterdam, 1968).
[3] J. Casas, N.M. Keita, and S.G. Steinemann, Phys. Chem. Liq. **14**, 155 (1984).
[4] J.P. Chan, Phys. Chem. Liq. **3**, 55 (1972).
[5] C.L. Prabhavathi, K. Siva Kumar, P. Venkateswarlu, and G.K. Raman, Phys. Chem. Liq. **38**, 705 (2000).
[6] U.N. Dash and B.K. Mohanty, Phys. Chem. Liq. **36**, 229 (1998).
[7] D. Ramachandran, K. Rambabu, P. Venkateswarlu, K. Mohankrishnan, and G.K. Raman, Phys. Chem. Liq. **33**, 1 (1996).
[8] H. Iloukhani and B. Samiey, Phys. Chem. Liq. **45**, 571 (2007).
[9] B.E. De Cominges, T.P. Iglesias, M.M. Pineiro, J.L. Legido, and M.I.P. Andrade, Phys. Chem. Liq. **37**, 673 (1999).
[10] H. Iloukhani, N. Zoorasna, and R. Soleimani, Phys. Chem. Liq. **43**, 391 (2005).
[11] S. Parthasarathy and N.N. Bakhshi, J. Phys. Chem. **57**, 453 (1952).
[12] J.D. Pandey, R. Dey, and B.D. Bhatt, J. Mol. Liq. **111**, 67 (2004).
[13] S. Blairs, J. Colloid Interf. Sci. **302**, 312 (2006).
[14] S. Magazu and G. Maisano, J. Mol. Liq. **93**, 7 (2001).
[15] R.T. Lagemann and W.S. Dunbar, J. Phys. Chem. **49**, 428 (1945).
[16] R.K. Shukla, S.K. Shukla, V.K. Pandey, and P. Awasthi, Phys. Chem. Liq. **45**, 169 (2007).

[17] M. Rastogi, A. Awasthi, and J.P. Shukla, Phys. Chem. Liq. **42**, 117 (2004).
[18] S. Goldman, J. Phys. Chem. **83**, 3033 (1979).
[19] E. Matteoli and G.A. Mansoori, J. Chem. Phys. **103**, 4672 (1995).
[20] A. Morsali, E.K. Goharshadi, G.A. Mansoori, and M. Abbaspour, Chem. Phys. **310**, 11 (2005).
[21] A. Morsali, E.K. Goharshadi, and N. Shahtahmasbi, Chem. Phys. **322**, 377 (2006).
[22] A. Morsali, S.A. Beyramabadi, and M.R. Bozorgmehr, Chem. Phys. **335**, 194 (2007).
[23] R.B. Stewart and R.T. Jacobsen, J. Phys. Chem. Ref. Data. **18**, 639 (1989).
[24] J. Kolafa and I. Nezbeda, Fluid Phase Equilibr. **100**, 1 (1994).
[25] A.D. Pierce, *Acoustics* (McGraw Hill, New York, 1981).